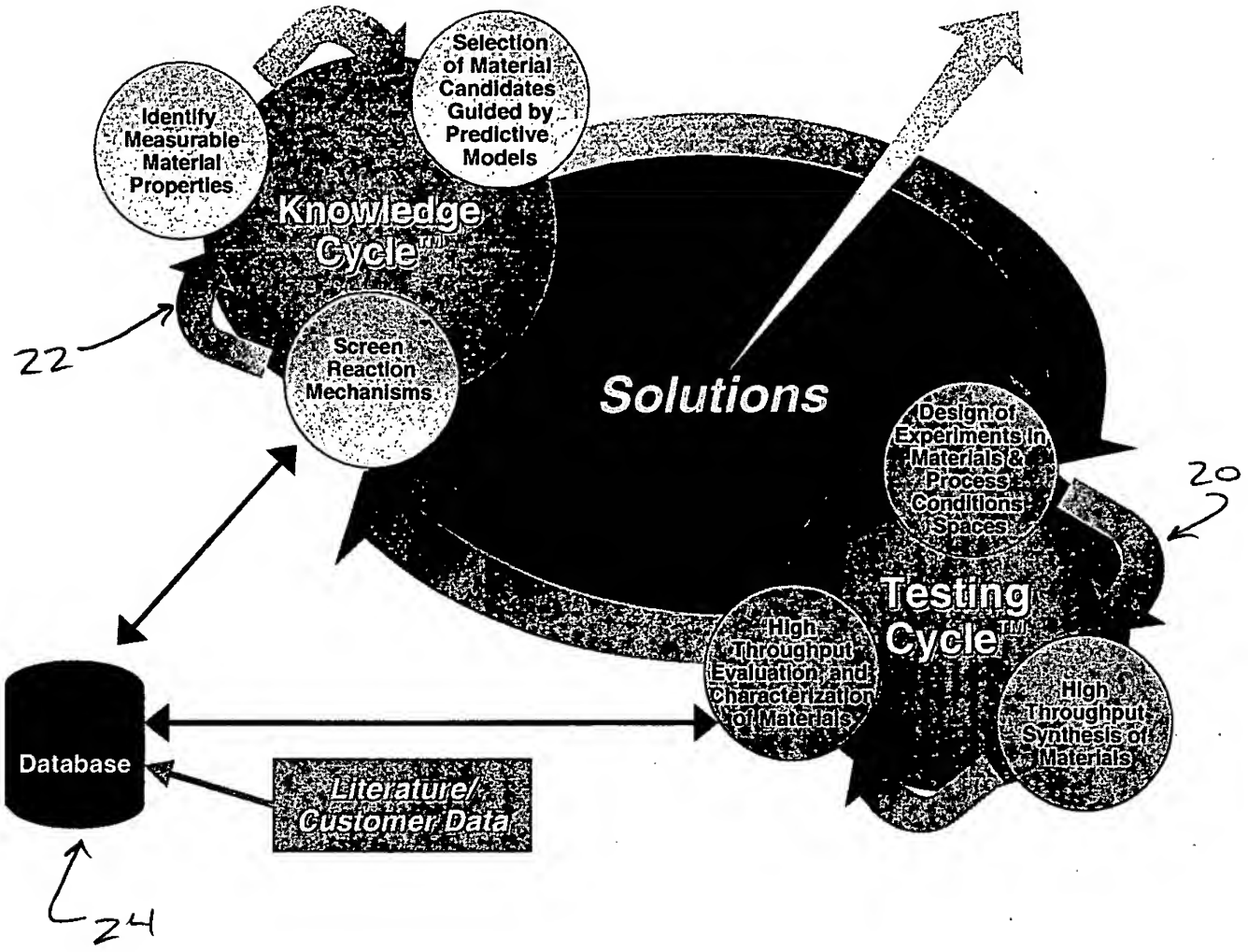
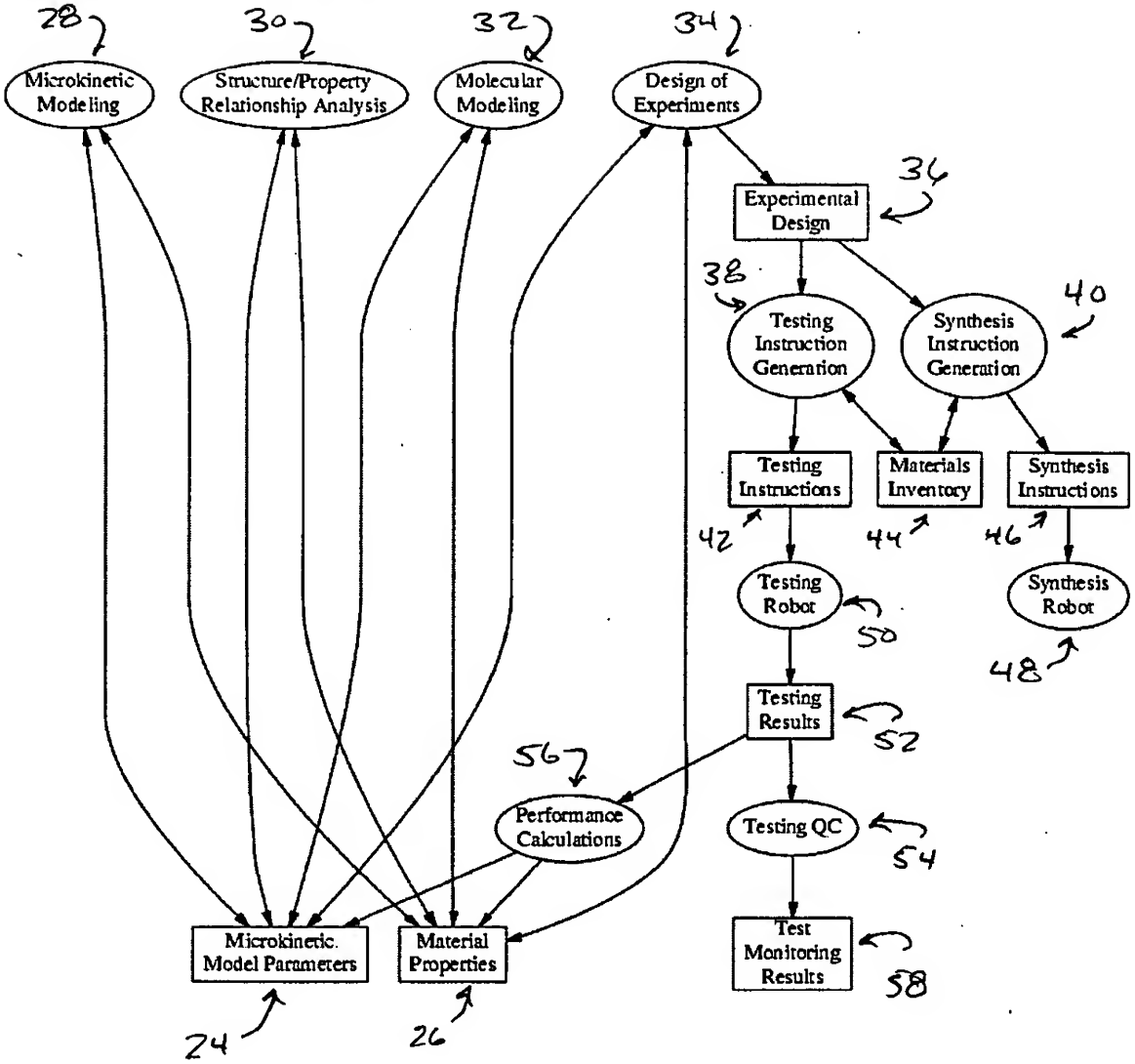


Fig. 1


28
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Microkinetic Modeling
Structure/Property Relationship Analysis
Molecular Modeling
Design of Experiments
Experimental Design
36
38
40
Testing Instruction Generation
Synthesis Instruction Generation
Testing Instructions
Materials Inventory
Synthesis Instructions
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46
Testing Robot
Synthesis Robot
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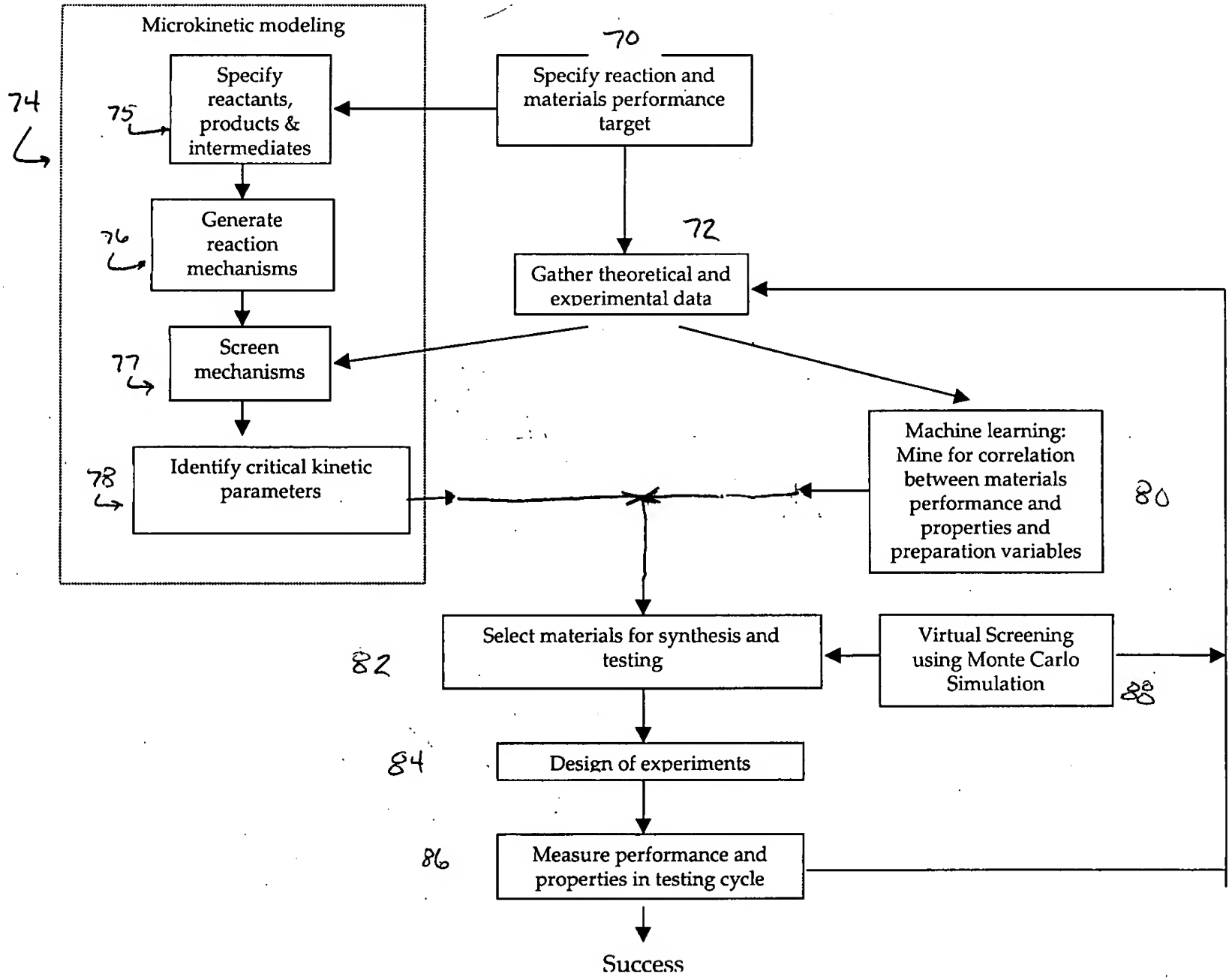
Testing Results
52
56
Performance Calculations
Testing QC
54
Test Monitoring Results
58
Microkinetic Model Parameters
Material Properties
24
26

Fig. 2.


Microkinetic modeling
74
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Specify reactants, products & intermediates
76
Generate reaction mechanisms
77
Screen mechanisms
78
Identify critical kinetic parameters
70
Specify reaction and materials performance target
72
Gather theoretical and experimental data
Machine learning: Mine for correlation between materials performance and properties and preparation variables
80
82
Select materials for synthesis and testing
Virtual Screening using Monte Carlo Simulation
88
84
Design of experiments
86
Measure performance and properties in testing cycle
Success

Fig. 3a

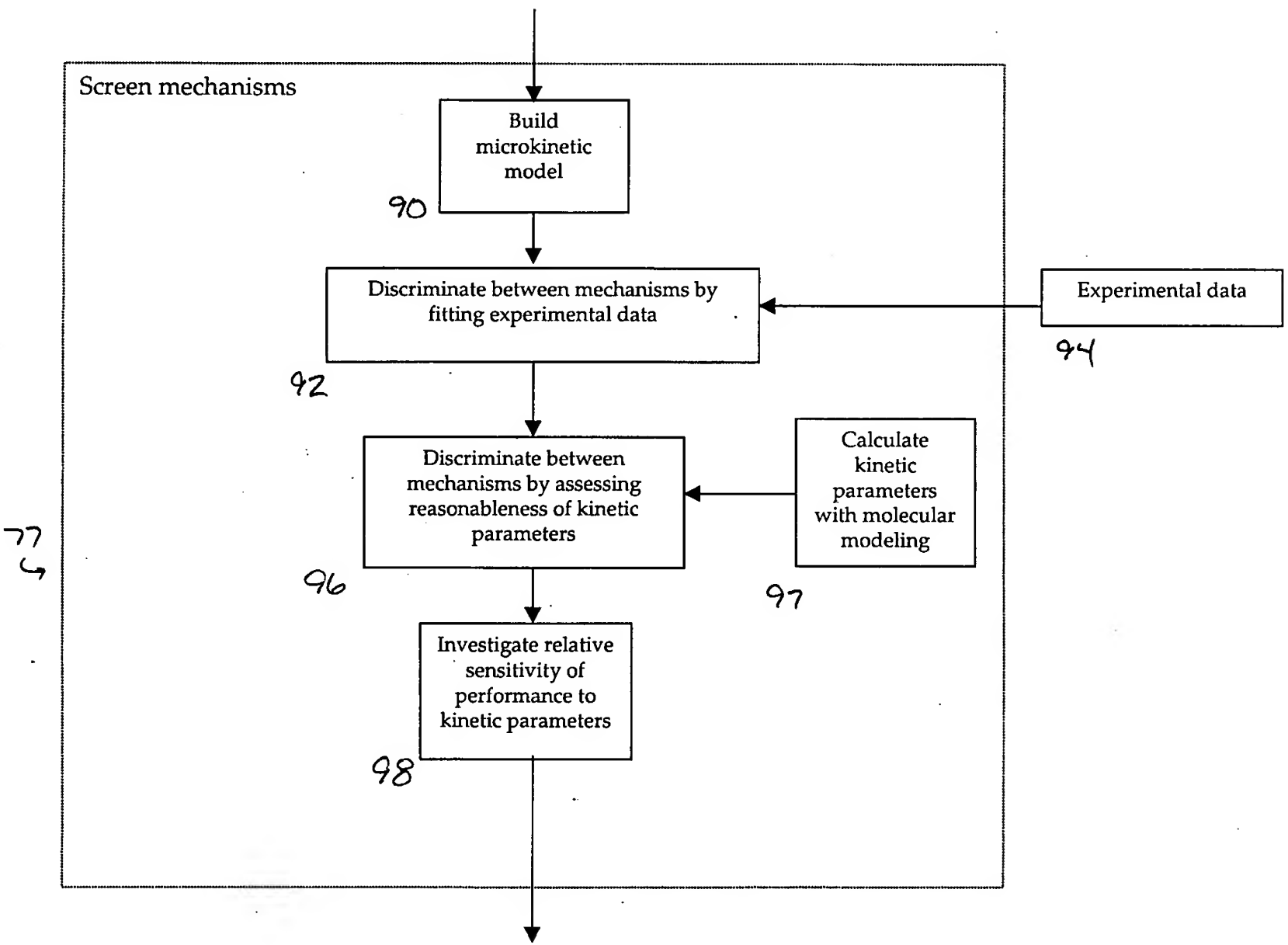
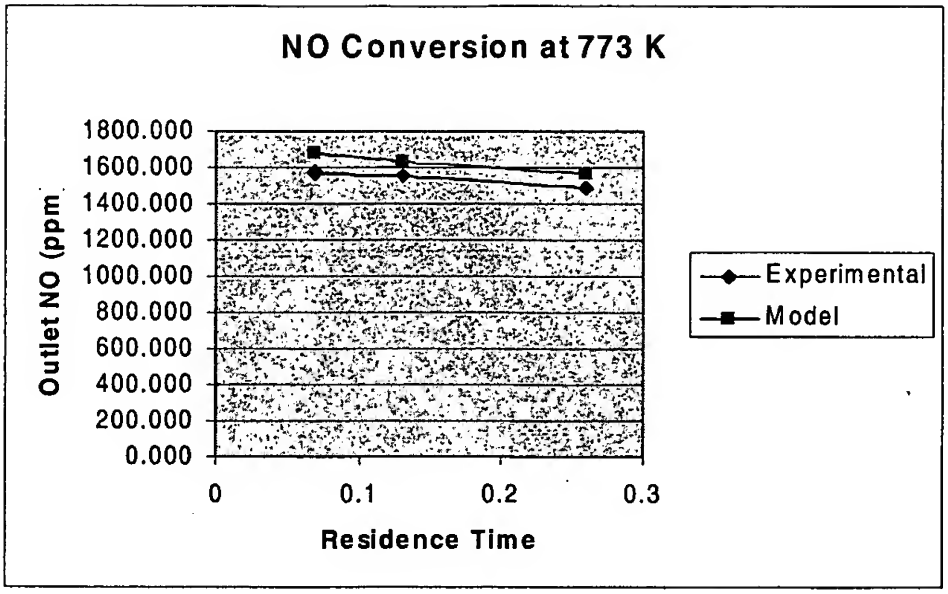
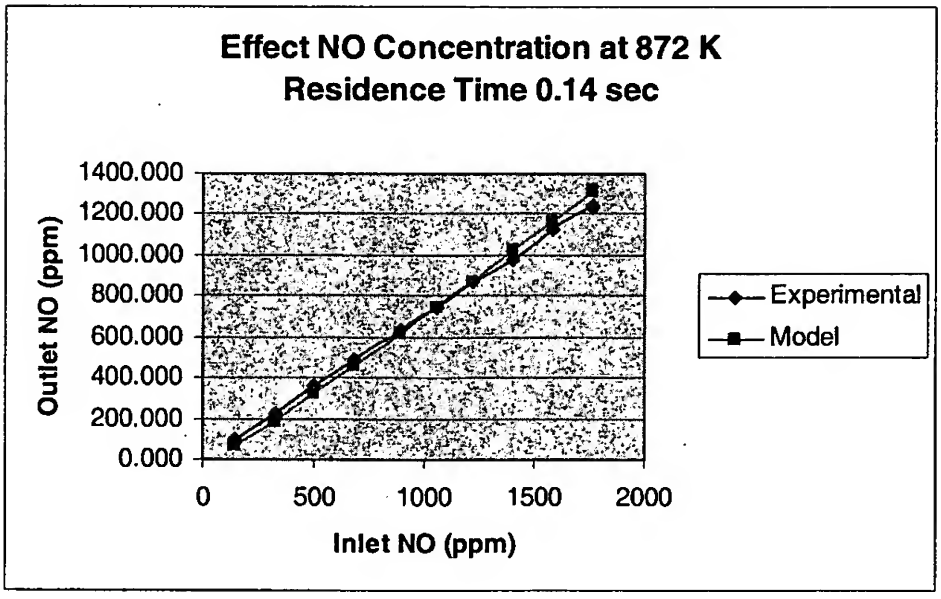

Screen mechanisms
Build microkinetic model
90
Discriminate between mechanisms by fitting experimental data
92
Experimental data
94
Discriminate between mechanisms by assessing reasonableness of kinetic parameters
96
Calculate kinetic parameters with molecular modeling
97
Investigate relative sensitivity of performance to kinetic parameters
98
77

Fig. 3b



Inlet NO Conc. =1760ppm

Fig. 4a



Reaction is first order in NO

Fig. 4b

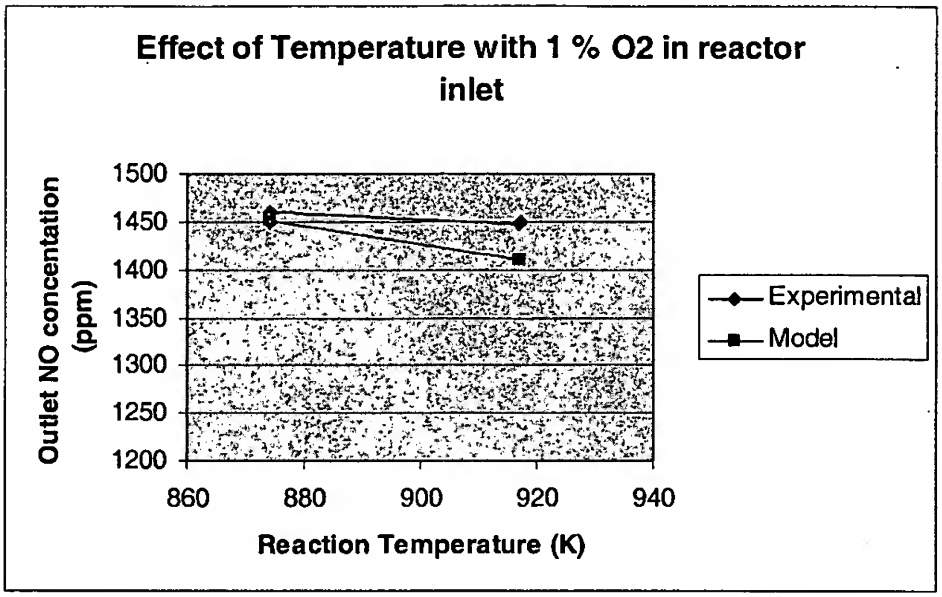


Fig. 4c

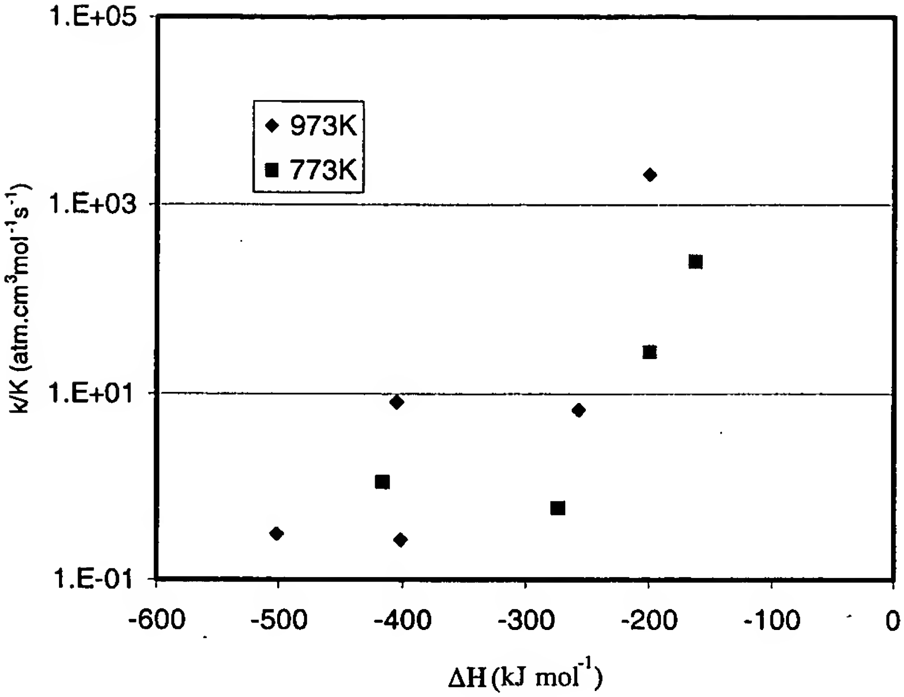

1.E+05
1.E+03
1.E+01
1.E-01
k/K (atm.cm^{3}mol^{-1}s^{-1})
973K
773K
-600
-500
-400
-300
-200
-100
0
ΔH (kJ mol^{-1})

Fig. 5

12291-101 C1

FIG. 6

X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	Y1	Y2
12	MgO	IIA	2800	38	35	1204.5	1.72	1.36	13.10	1.31	7.646	0.2260	1.560	10.60	1.736	1.756	1.662	0.110	cubic	26.24	37
13	Al_2O_3	IIIA	2046.7	45	43	1117.0	1.82	1.18	16.50	1.61	5.986	0.3770	2.370	6.80	1.643	3.678	1.191	0.137	hexagonal	24.90	38
20	CaO	IIA	2587	30	34	1271.0	2.23	1.74	40.00	1.00	6.113	0.2980	2.000	22.80	1.837	2.886	2.416	0.088	cubic	27.01	28
21	Sc_2O_3	IIIB	2405	43	46	1147.2	2.09	1.44	315.00	1.36	6.540	0.0177	0.158	17.80	1.99	7.020	2.149	0.064	cubic	29.17	31
22	TiO_2	IVB	1855	35	39	941.6	2.00	1.32	153.00	1.54	6.820	0.0234	0.219	14.60	2.616	4.931		0.021	Rutile	25.86	19
24	Cr_2O_3	VIB	2300	38	40	753.6	1.85	1.18	180.00	1.66	6.766	0.0774	0.937	11.60	2.5	7.352	2.251	0.026	hexagonal	24.16	23
26	Fe_2O_3	VIII	1562	27	22	548.5	1.72	1.17		1.83	7.870	0.0993	0.802	8.40	2.95	8.685	2.695	0.013	hexagonal	25.31	16
28	NiO	VIII	1957	45	39.5	489.0	1.62	1.15		1.91	7.635	0.1430	0.907	6.80	2.37	2.407		0.032	cubic	29.12	30
29	CuO	IB	1336	22	24	310.7	1.57	1.17	-5.46	1.90	7.726	0.5960	4.010	6.10	2.84	3.455		0.015		28.91	9
30	ZnO	IIB	1975	36	42	696.7	1.53	1.25	-11.40	1.65	9.394	0.1660	1.160	7.10	2.004	2.882	2.382	0.062	hexagonal	25.38	41
31	Ga_2O_3	IIIA	1740	40.5	40.5	720.1	1.81	1.26	-21.60	1.81	5.999	0.0678	0.406	8.12	1.935	5.506		0.071	hexagonal	24.93	29
38	SrO	IIA	2430	15	23	1282.8	2.45	1.91	92.00	0.95	5.695	0.0762	0.353	27.60	1.87	3.966	3.106	0.082	cubic	31.37	15
39	Y_2O_3	IIIB	2376	18.5	27.5	1172.3	2.27	1.62	187.70	1.22	6.380	0.0166	0.172	22.70	1.91	8.662	2.521	0.075	cubic	28.14	24
45	Rh_2O_3	VIII	1115	10	34	190.6	1.83	1.25	111.00	2.28	7.460	0.2110	1.500	8.60					rhombic	29.81	14
50	SnO_2	IVA	1625	27	32	581.1	1.72	1.41	-37.00	1.96	7.344	0.0917	0.666	7.70	1.997	4.284		0.063	tetragonal	25.89	19
57	La_2O_3	IIIB	2300	11	20	1199.3	2.74	1.69	95.90	1.10	5.580	0.0126	0.135	31.10					hexagonal	28.54	16
58	CeO_2	LANT	2397	26	26	1089.3	2.70	1.65	2500.00	1.12	5.540	0.0115	0.114	29.60					cubic	27.75	18
60	Nd_2O_3	LANT	2315	12	28	1206.2	2.64	1.64	5930.00	1.14	5.530	0.0157	0.165	31.40						28.67	25
62	Sm_2O_3	LANT	2320	19	23	1211.1	2.59	1.62	1860.00	1.17	5.640	0.0096	0.133	30.10	2.100	9.927		0.051		28.42	14
63	Eu_2O_3	LANT	2330	16	27.5	1156.4	2.56	1.85	30900.00	1.20	5.670	0.0112	0.139	28.80	2.105	10.047		0.051	cubic	27.84	23
64	Gd_2O_3	LANT	2395	12	26.5	1211.2	2.54	1.61	185000.00	1.20	6.150	0.0074	0.106	27.70	2.093	10.265		0.052	cubic	27.24	19
66	Dy_2O_3	LANT	2385	18	36	1244.4	2.49	1.59	98000.00	1.22	5.940	0.0108	0.107	24.50	2.041	10.236		0.058	cubic	28.62	25
67	Ho_2O_3	LANT	2395	37	40	1253.8	2.47	1.58	72900.00	1.23	6.018	0.0124	0.162	23.60	1.960			0.068	cubic	29.55	32.5
68	Er_2O_3	LANT	2400	36	39.5	1265.3	2.45	1.57	48000.00	1.24	6.101	0.0117	0.143	22.70	1.950	27.611		0.069	cubic	26.43	28
69	Tm_2O_3	LANT	2425	34	32	1259.4	2.42	1.56	24700.00	1.25	6.184	0.0150	0.168	21.80	1.950			0.069	cubic	27.35	28
70	Yb_2O_3	LANT	2420	30	32	1210.0	2.40	1.74	67.00	1.10	6.254	0.0351	0.349	21.00	1.940	8.160		0.071	cubic	26.15	29
71	Lu_2O_3	LANT	2467	29	35	1252.1	2.25	1.56		1.27	5.430	0.0185	0.164	21.90	1.930	7.962		0.072		27.81	26
72	HfO_2	IVB	2790	30	30	1113.7	2.16	1.44	75.00	1.30	6.650	0.0312	0.230	16.20	2.000	4.164		0.063	monoclinic	25.79	18
77	IrO_2	VIII	1100	24	30.5	184.2	1.87	1.27	25.60	2.20	9.100	0.1970	1.470	7.60					tetragonal	32.01	16
90	ThO_2	ACTI	3300	22	30	1227.6		1.65	132.00	1.30	6.080	0.0653	0.540	32.10	2.200	5.870		0.043	cubic	26.51	14

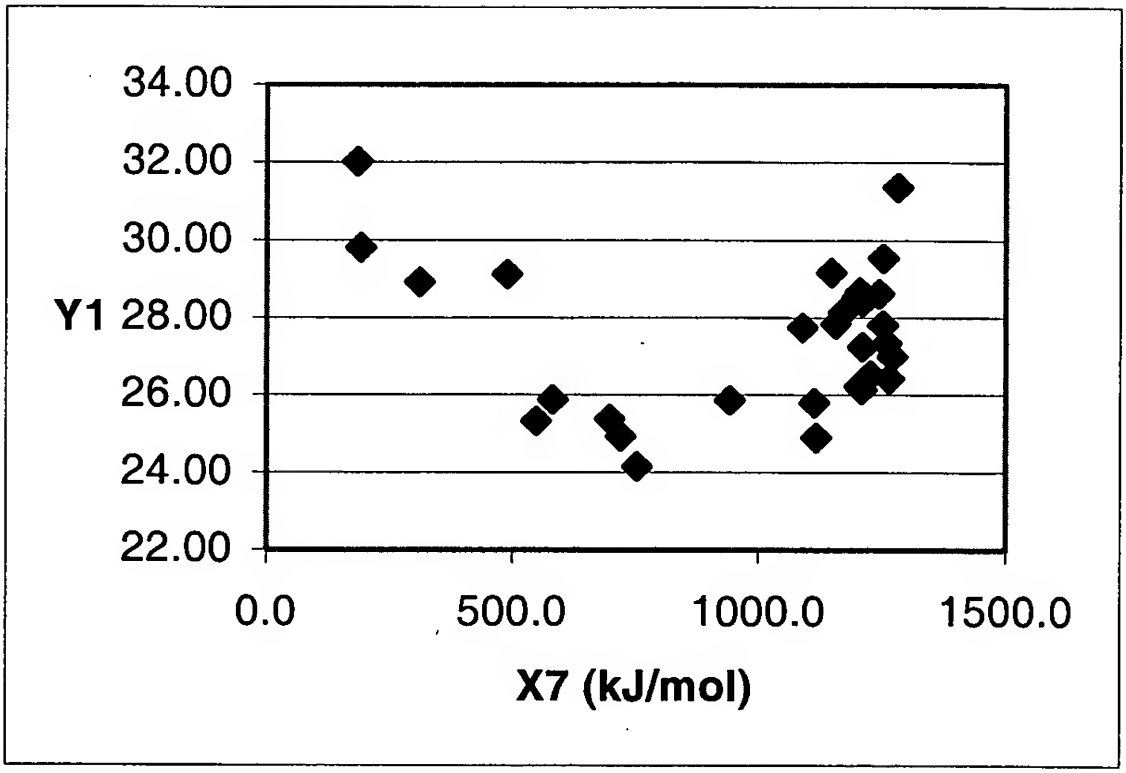


Fig. 7

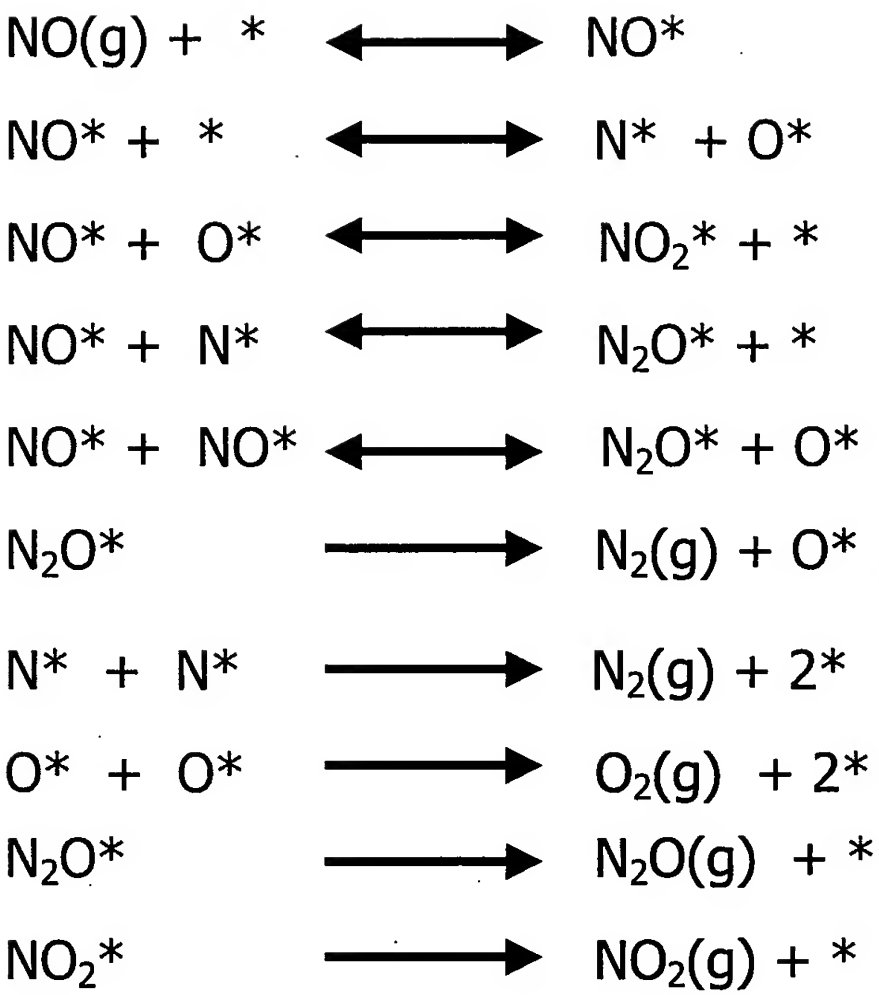

NO(g) + * ⟷ NO*
NO* + * ⟷ N* + O*
NO* + O* ⟷ NO2* + *
NO* + N* ⟷ N2O* + *
NO* + NO* ⟷ N2O* + O*
N2O* → N2(g) + O*
N* + N* → N2(g) + 2*
O* + O* → O2(g) + 2*
N2O* → N2O(g) + *
NO2* → NO2(g) + *

Fig. 8

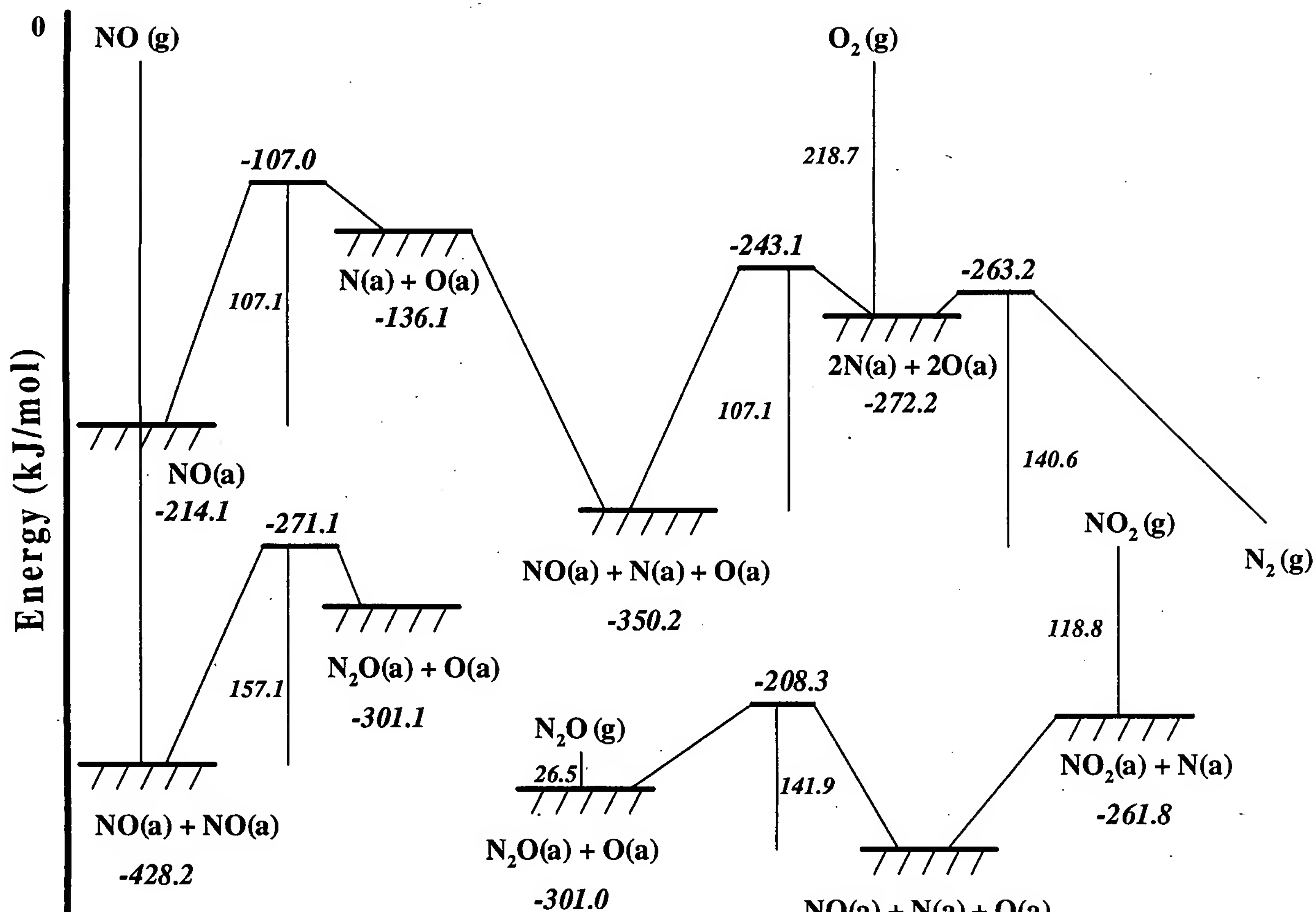
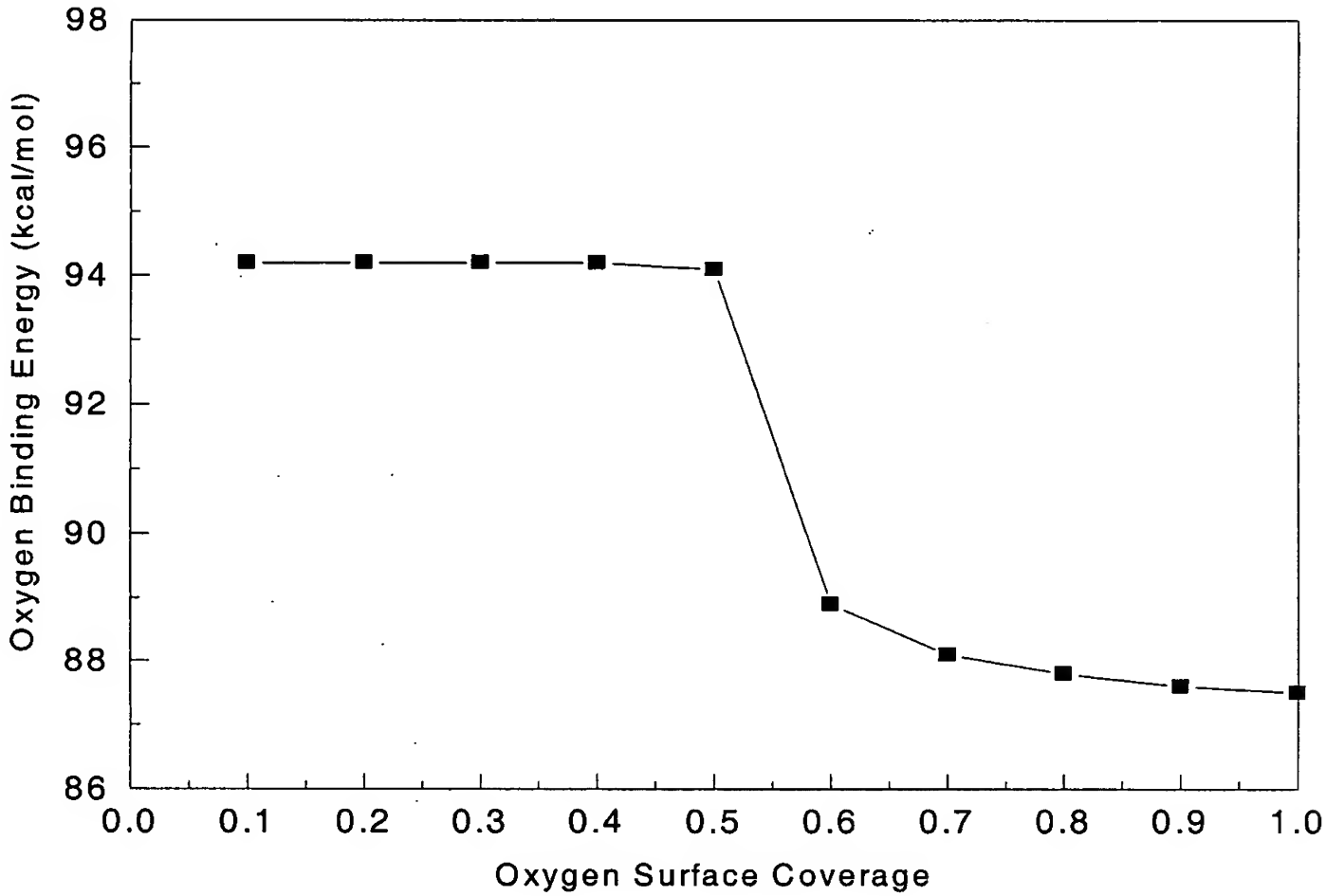

0
Energy (kJ/mol)
NO (g)
-107.0
107.1
N(a) + O(a)
-136.1
NO(a)
-214.1
-271.1
157.1
N₂O(a) + O(a)
-301.1
NO(a) + NO(a)
-428.2
NO(a) + N(a) + O(a)
-350.2
-243.1
107.1
O₂ (g)
218.7
2N(a) + 2O(a)
-272.2
-263.2
140.6
N₂ (g)
N₂O (g)
26.5
N₂O(a) + O(a)
-301.0
-208.3
141.9
NO(a) + N(a) + O(a)
-350.2
NO₂ (g)
118.8
NO₂(a) + N(a)
-261.8

Fig. 7

FIG. 9


Oxygen Binding Energy (kcal/mol)
98
96
94
92
90
88
86
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Oxygen Surface Coverage

1

Fig. 10

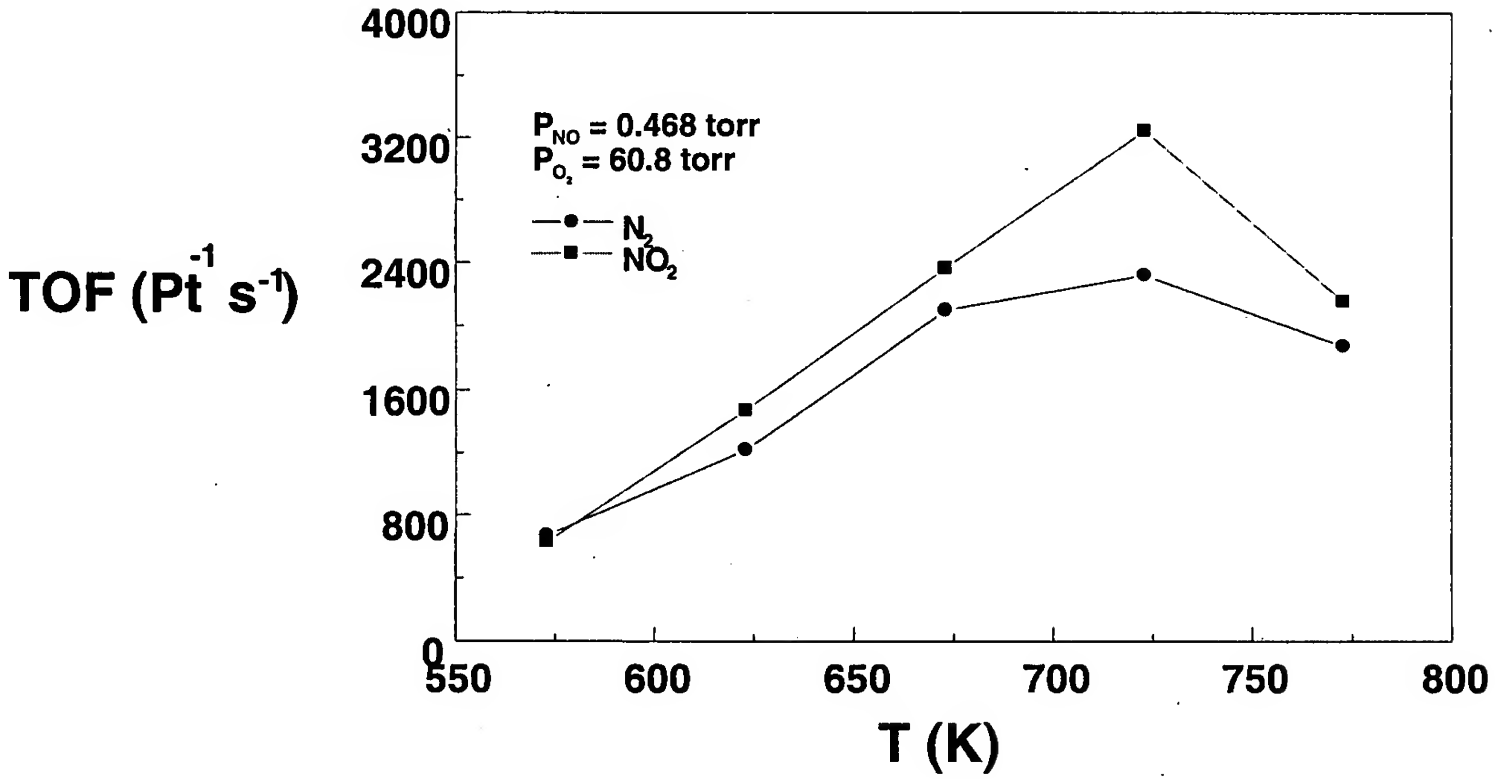

TOF (Pt^{-1} s^{-1})
4000
3200
2400
1600
800
0
550
600
650
700
750
800
T (K)
P_{NO} = 0.468 torr
P_{O_2} = 60.8 torr
N_2
NO_2

Fig. 11

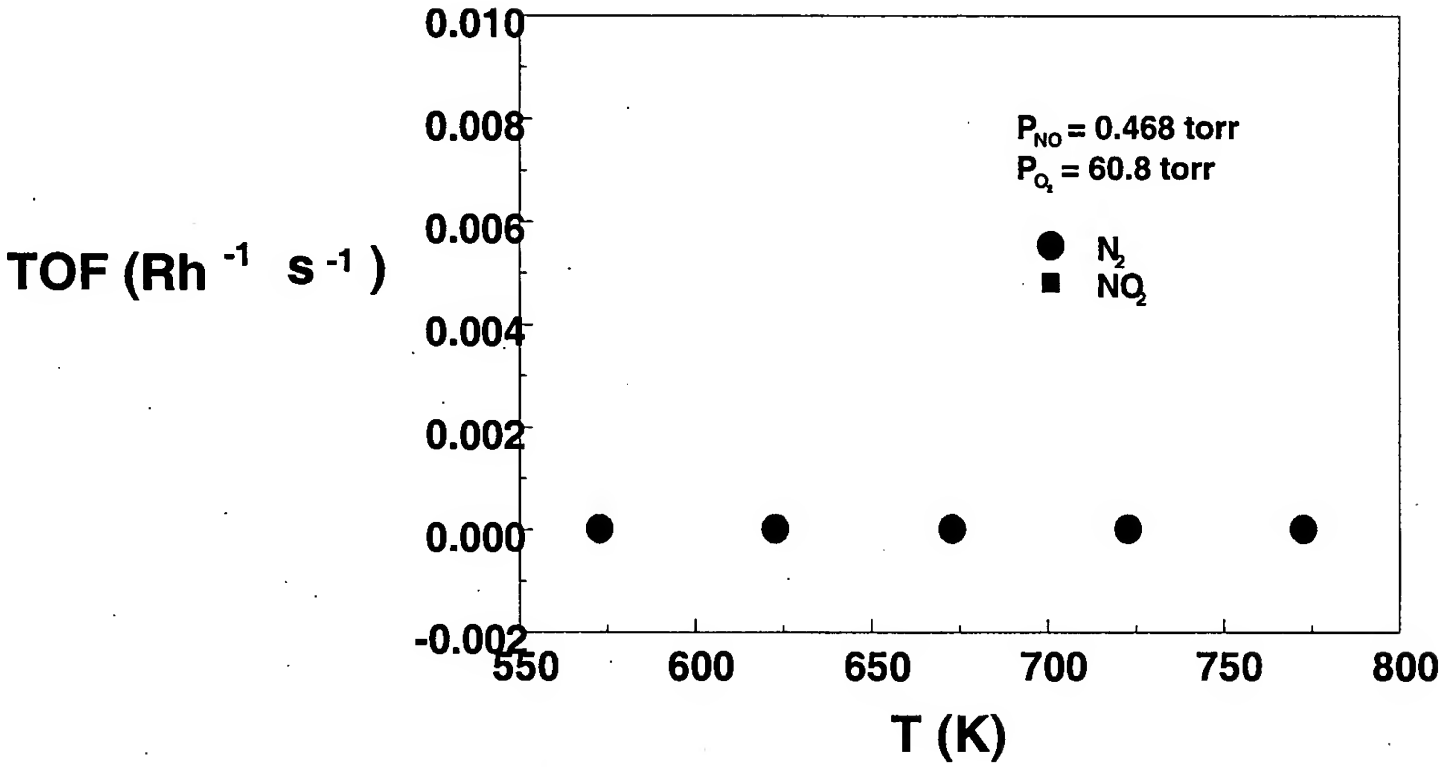

TOF (Rh -1 s -1)
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
550
600
650
700
750
800
T (K)
P NO = 0.468 torr
P O2 = 60.8 torr
N2
NO2

Fig. 12

Periodic Trends in Chemisorption and Activation Energies

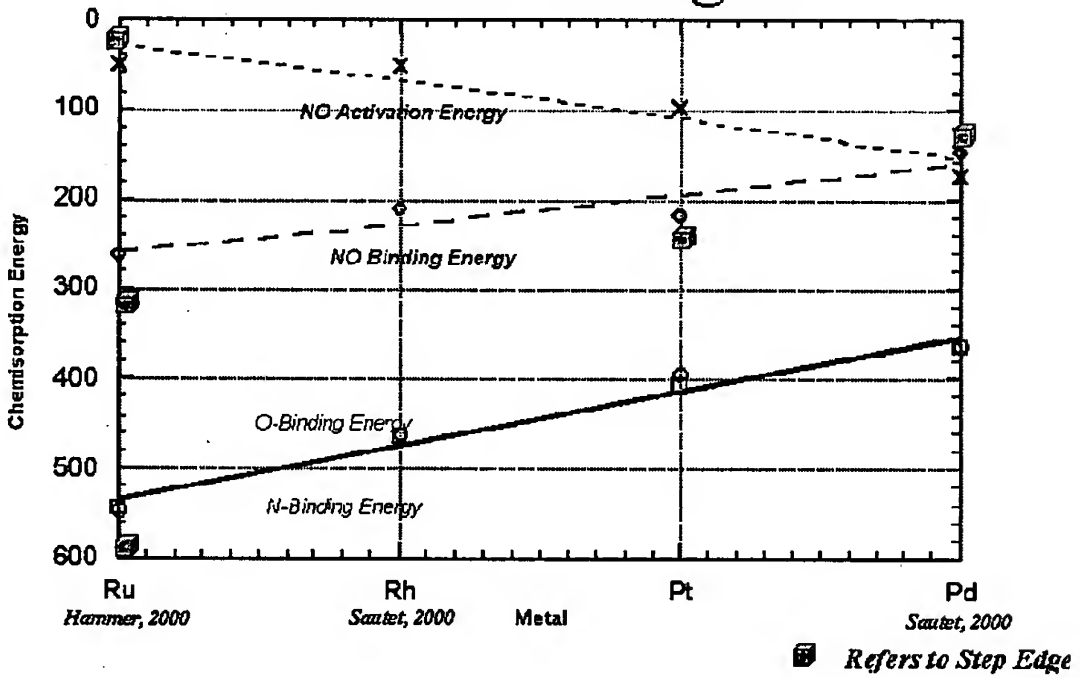


Fig. 13

Structure Sensitivity for NO Decomposition

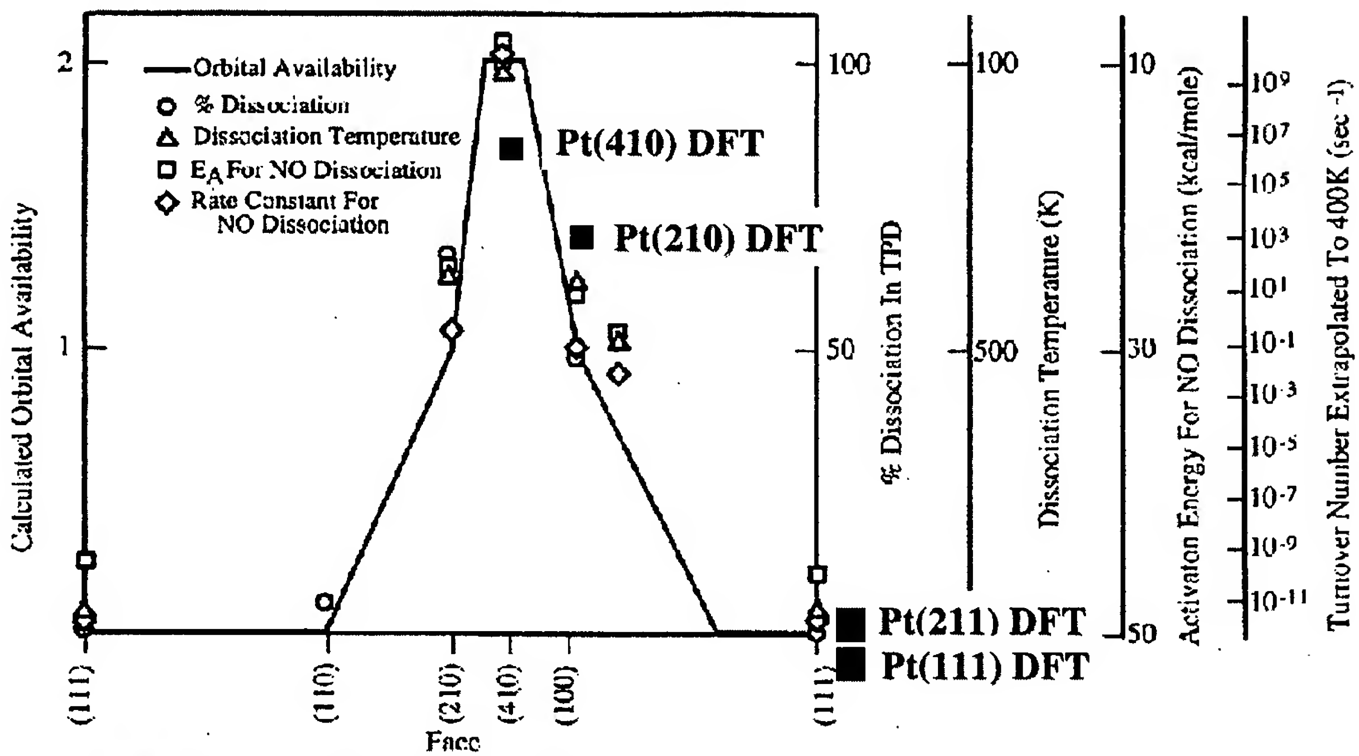


Figure 6.14 The rate on nitric oxide dissociation on several of the faces of platinum along the principle zone axes of the stereographic triangle. (Adapted from Masel [1983].)

Fig. 14

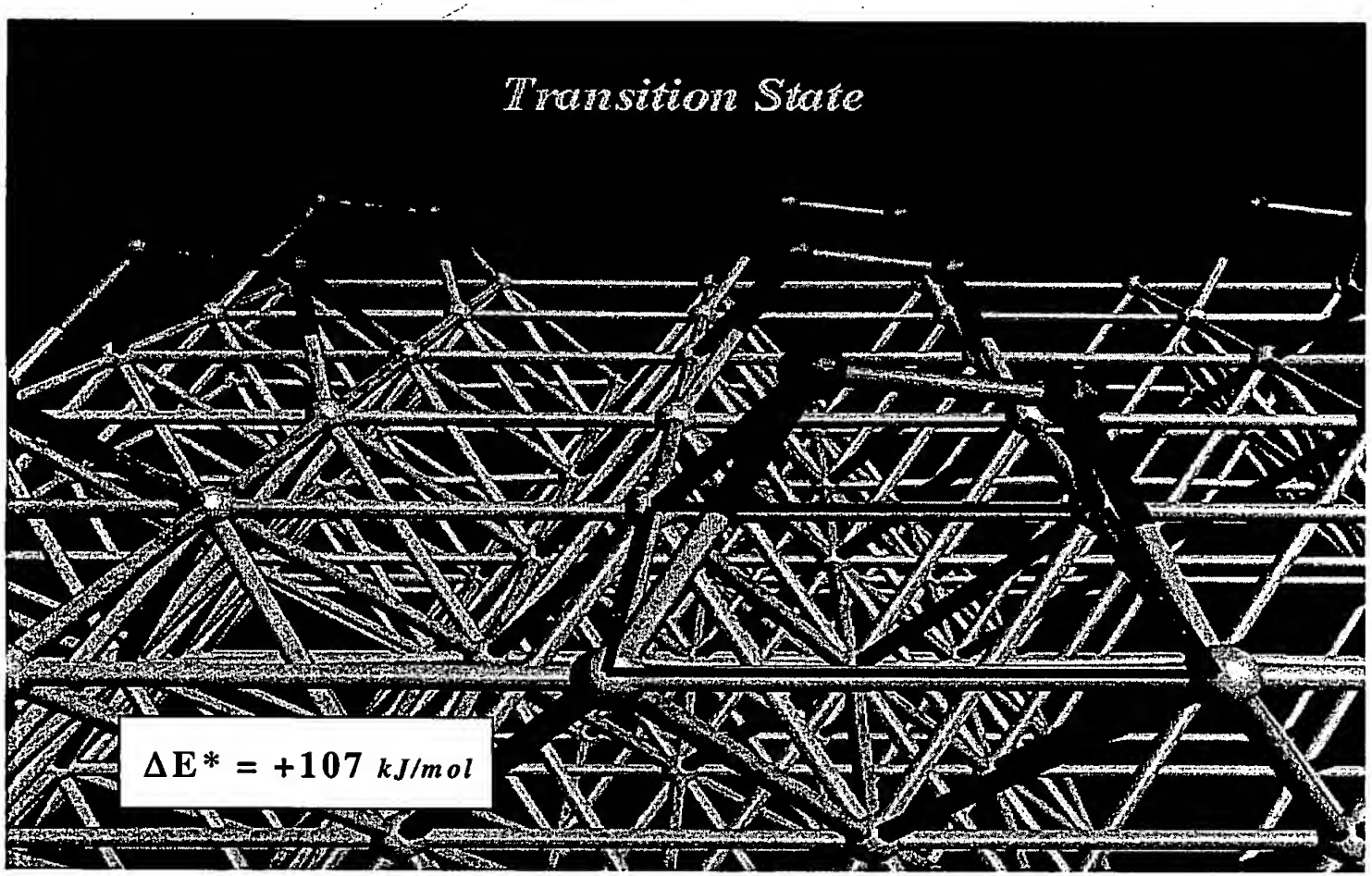


Fig. 15

FIG. 16 Representative Computer

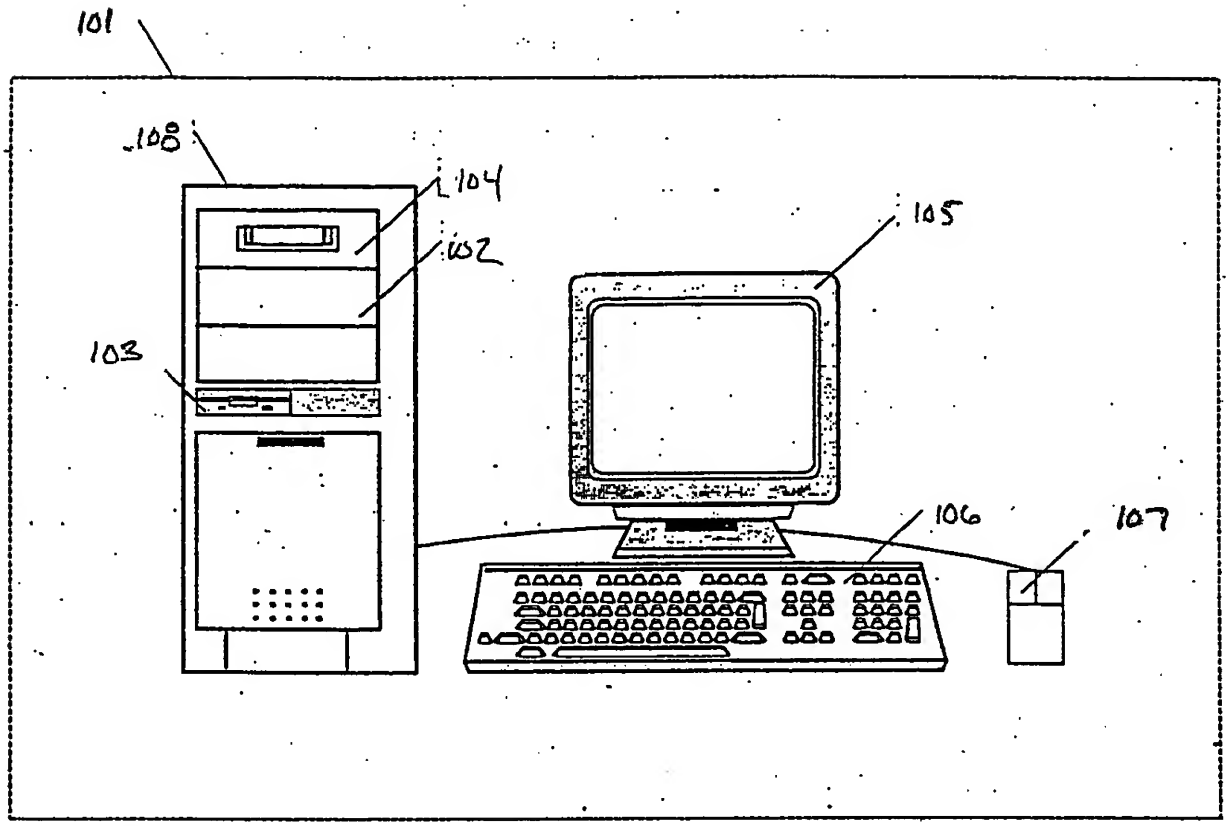


FIG 1 Computer System Internal Diagram